2.4 Schrödinger's wave equation

- In Schrödinger picture, now we know

$$i\hbar \frac{\partial}{\partial t} |\alpha, t_0; t\rangle = H |\alpha, t_0; t\rangle$$

for a general quantum state $|\alpha\rangle$.

let $t_0 = 0$, the x-representation becomes

$$\langle \vec{x}| \cdot (\quad) \Rightarrow i\hbar \frac{\partial}{\partial t} \langle \vec{x}|\alpha, t\rangle = \langle \vec{x}|H|\alpha, t\rangle$$

- For $H = \frac{\tilde{\vec{p}}^2}{2m} + V(\underset{\sim}{\vec{x}})$,

$$i\hbar \frac{\partial}{\partial t} \langle \vec{x}|\alpha, t\rangle = -\frac{\hbar^2}{2m} \nabla^2 \langle x|\alpha, t\rangle + V(\vec{x}) \langle x|\alpha, t\rangle .$$

Letting $\psi(\vec{x}, t) \equiv \langle \vec{x}|\alpha, t\rangle$, (wave function)

$$i\hbar \frac{\partial}{\partial t} \psi(\vec{x}, t) = \left[-\frac{\hbar^2}{2m} \nabla^2 + V(\vec{x}) \right] \psi(\vec{x}, t)$$

: This is what you've seen in the undergraduate course.

- If $|\alpha\rangle = |a\rangle$ (energy eigenstate)

$$|a, t\rangle = U(t)|a\rangle = e^{-\frac{i}{\hbar}Ht}|a\rangle = e^{-\frac{iE_a t}{\hbar}}|a\rangle .$$

Thus, $\left[-\frac{\hbar^2}{2m} \nabla^2 + V \right] u_E(\vec{x}) = E\, u_E(\vec{x})$

where $\langle \vec{x}|a\rangle = u_E(\vec{x})$ ... Energy - Eigenfunction.

$\Rightarrow$ time-independent Schrödinger equation.

← P.D.E, solvable under boundary conditions.

$u_E(x)$: bounded ($u_E \to 0$ as $|x| \to \infty$) ⇒ discrete E (quantized!)

unbounded → continuous E.

• "Semi-classical" solution : WKB approximation.

(Wentzel, Kramers, Brillouin)

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{x})\right] u_E(\vec{x}) = E\, u_E(\vec{x})$$

1D

$$\Rightarrow \quad \frac{d^2 u_E(x)}{dx^2} + (k(x))^2\, u_E(x) = 0$$

$k(x) = \sqrt{\frac{2m}{\hbar^2}(E - V(x))}$ for $E > V(x)$

$k(x) = -i\sqrt{\frac{2m}{\hbar^2}(V(x) - E)}$ for $E < V(x)$

Try a solution of the form

$$u_E(x) = \exp\left[\, i W(x)/\hbar \,\right]$$

exact when $V(x) = $ constant.

$$\Rightarrow \quad i\hbar \frac{d^2W}{dx^2} - \left(\frac{dW}{dx}\right)^2 + \hbar^2 [k(x)]^2 = 0.$$

★★★

so far, it's still exact.

★ Approximation for a "slowly varying" potential,

$$\Leftrightarrow \quad \hbar \left|\frac{d^2W}{dx^2}\right| \ll \left|\frac{dW}{dx}\right|^2$$

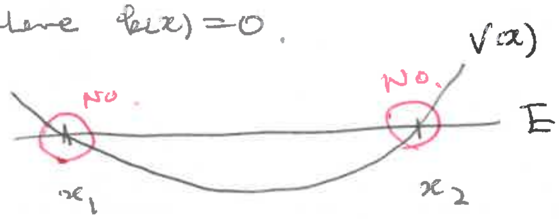
How are they related? - NOT OBVIOUS!

→ $\left(i\hbar \frac{d^2W}{dx^2}\right)$ term is smaller than others. ($|k| \gg 1$).

‖ far from the turning points where $k(x) = 0$.

• Iterative solution

$$\Rightarrow \quad \frac{dW}{dx} = \pm \hbar k(x)$$



$$\Rightarrow \quad W_0 = \pm \int^x dx' \, \hbar k(x')$$

(zeroth order).

first-order: $$\left(\frac{dW}{dx}\right)^2 = \hbar^2[k(x)]^2 + i\hbar\frac{d^2W_0}{dx^2}$$
$$= \hbar^2 k^2 \pm i\hbar^2 k'$$

$$\Rightarrow \quad W(x) \simeq \pm\hbar\int^x dx'\,\left[k^2(x') \pm i k'(x')\right]^{1/2}$$

since $k' \ll k^2$ $\quad\left(\hbar\left|\frac{d^2W}{dx^2}\right| \ll \left|\frac{dW}{dx}\right|^2\right)$

$$W(x) \simeq \pm\hbar\int^x dx'\,k(x')\left[1 \pm \frac{1}{2}\cdot i\,\frac{k'}{k^2}\right]$$

$$= \pm\hbar\int^x dx'\,k(x') + \frac{i}{2}\hbar\ln[k(x)]$$

$$\therefore \quad u_E(x) \simeq \exp[iW(x)/\hbar]$$
$$\simeq \frac{1}{[k(x)]^{1/2}}\exp\left[\pm i\int^x dx'\,k(x')\right]$$

linear combination of these.

- meaning of a "slowly varying" potential.

$$\hbar\left|\frac{d^2W}{dx^2}\right| \ll \left|\frac{dW}{dx}\right|^2 \xrightarrow{\text{zeroth order}} k' \ll k^2$$

$$\Rightarrow \frac{1}{2\hbar}\sqrt{2m}\,\frac{1}{\sqrt{(E-V(x))}}\cdot\left|\frac{dV}{dx}\right| \ll \frac{2m}{\hbar^2}[E-V(x)]$$

$$\Rightarrow \quad \frac{\hbar}{\sqrt{2m(E-V)}} \ll \frac{2[E-V]}{\left|\frac{dV}{dx}\right|}$$

$\hbar/p$

$\Downarrow$

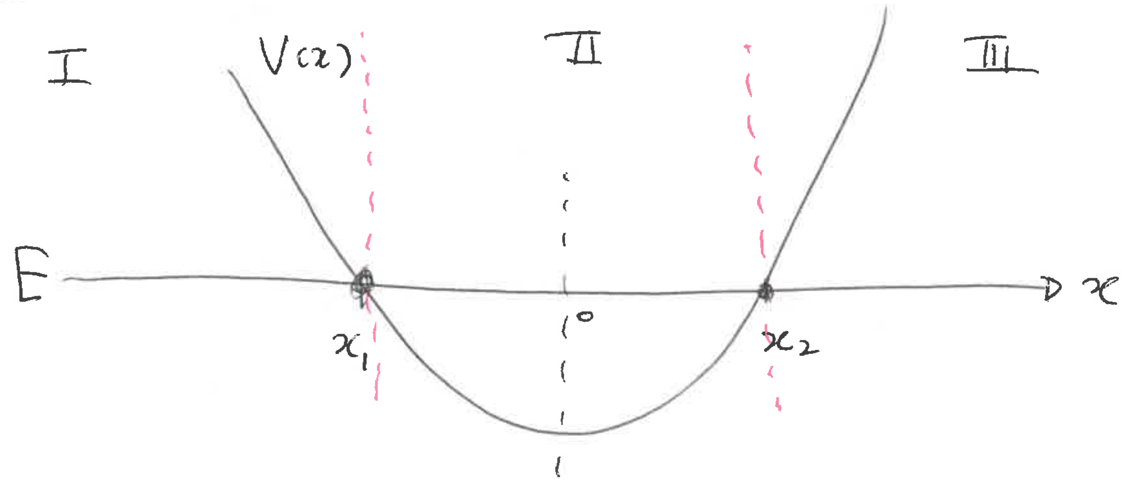
"Slowly varying V" $\Leftrightarrow$ "Short wavelength"

$$\boxed{\frac{\lambda}{2\pi} \ll \text{characteristic distance over which the potential varies appreciably.}}$$

But, why it's "semi-classical"?

— We will see this later...

- **Matching**: connection formula



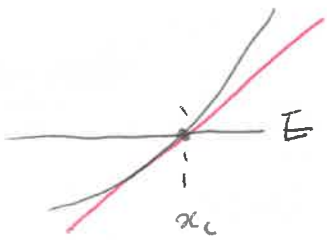
WKB approx.: Good when $E > V(x)$ or $E < V(x)$

BAD around x_1 and x_2 (turning points).

How can we find a proper $u_E(x)$ that are valid in I, II, III regions?

→ Asymptotic behavior of $u_E(x)$.

approx. of $V(x)$ → linear potential at $x \approx x_c$.



$$V(x) = V(x_c) + V'(x_c)(x - x_c) + \cancel{\cdots}$$

⇓ Schrödinger eq.

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V'(x_c)(x - x_c)\psi = 0$$

|| NOTE: $E = V(x_c)$.

$$\Rightarrow \frac{d^2 y}{dz^2} - zy = 0 \quad \Bigg| \quad \begin{aligned} y &= \psi \\ z &= \left(\frac{2m V'(x_c)}{\hbar^2}\right)^{\frac{1}{3}} (x - x_c) \end{aligned}$$

Try $\quad y(z) = \int_C F(s) e^{sz} ds \quad \cdots$ complex ver. of Laplace transformation.

$$\Rightarrow \int_C (s^2 - z) F(s) e^{sz} ds = 0.$$

$\Rightarrow \frac{d}{dz}(e^{sz})$

Doing Integration by parts,

$$\left[-F(s) e^{sz} \right]_C + \int_C \left(s^2 F + \frac{dF}{ds} \right) e^{sz} dz = 0.$$

$\Rightarrow$ Two conditions :

① $\left[-F(s) e^{sz} \right]_C = 0$: Choose the contour "C" s.t. $[\ \ ]_C = 0$.

② $\frac{dF}{ds} + s^2 F = 0 \Rightarrow F(s) \propto e^{-\frac{1}{3}s^3}$

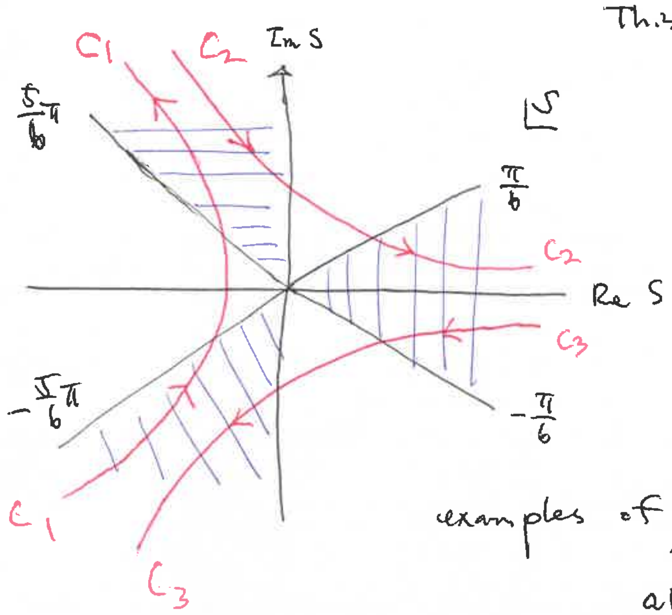
$$\to \left[F(s) e^{sz} \right]_C = \left[e^{-\frac{1}{3}s^3 + sz} \right]_C = 0.$$

This has to vanish at the endpoints of C. i.e. $\left| e^{-\frac{s^3}{3}} \right| \to 0$

$\downarrow$

" $\cos 3\theta > 0$. "

where $s = re^{i\theta}$



examples of "C".

allowed.

⇒ general solutions

$$Ai(z) = \frac{1}{2\pi i}\int_{C_1} e^{sz - \frac{s^3}{3}}\, ds \quad \cdots \text{ Airy function}$$

$$Bi(z) = \frac{1}{2\pi}\left[\int_{C_2} e^{sz-\frac{s^3}{3}}\, ds - \int_{C_3} e^{sz-\frac{s^3}{3}}\, ds\right]$$

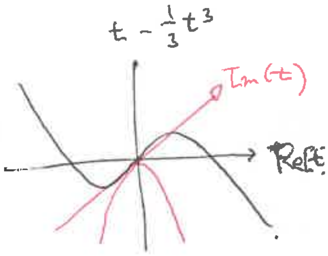
... the second kind.

- Asymptotic behaviors

① $z \to \infty$

Let $s = z^{\frac{1}{2}} t$, $\quad (ds = z^{\frac{1}{2}} dt)$

$$Ai(z) = \frac{1}{2\pi i} z^{\frac{1}{2}} \int_{C_1} e^{z^{\frac{3}{2}}\left(t - \frac{1}{3}t^3\right)} dt.$$



(aka. method of steepest descent)

→ Saddle-point approximation

$$\leq \frac{1}{2\pi i} z^{\frac{1}{2}} \int_{C_1} e^{z^{\frac{3}{2}} \cdot \underbrace{Y_0\left[t - \frac{1}{3}t^3\right]}_{\text{saddle point}}} dt$$

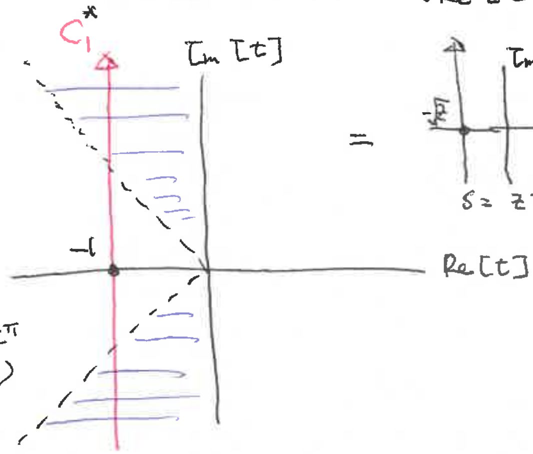
since $|z|$ is large it goes to "$\simeq$"

$\downarrow$ $\nabla_t Y_0 = 0$

at $t = -1$.

NOTE
$Re[s] < 0$
$(Re[t]$ in C_1

Thus, choose C_1 as



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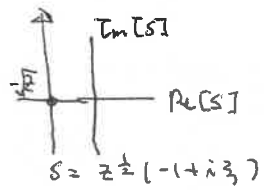

$t = -1 + i\xi$ (the most rapid decrease at $\arg[t] = \frac{1}{2}\pi$ or $\frac{3}{2}\pi$ (see Arfken)

$$\Rightarrow t - \frac{1}{3}t^3$$

$$\approx -\frac{2}{3} - \xi^2 + O(\xi^3)$$

$$Ai(z) \simeq \frac{1}{2\pi i} z^{\frac{1}{2}} \cdot i \int_{-\infty}^{+\infty} d\xi\; e^{z^{\frac{3}{2}}\left(-\frac{2}{3} - \xi^2\right)}$$

$$= \frac{1}{2\sqrt{\pi}} |z|^{-\frac{1}{4}} \exp\left[-\frac{2}{3}|z|^{\frac{3}{2}}\right] \quad \text{as } z \to \infty.$$

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